HyPEP Model Development

Chang Oh, Steven Sherman

Idaho National Laboratory

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Project ID # PDP29

Overview

Timeline

- Start: October 2005
- End: September 2008
- Percent complete: 55%

Barriers

- High-temperature thermochemical technology
- Technology-validation – hydrogen from nuclear power

Budget

- Total project funding
  - DOE share: $1,270K
  - Partner share: $300K
- Funding received in FY06: $390K
- Funding for FY07: $530K

Partners

- Idaho National Laboratory (INL)
- Argonne National Laboratory (ANL)
- Korea Atomic Energy Research Institute (KAERI)

Objectives

- HyPEP – <u>Hy</u>drogen <u>P</u>roduction <u>E</u>fficiency Calculation <u>P</u>rogram
- Overall
  - Development of an easy-to-use, non-proprietary, fast-running software tool for evaluating and optimizing nuclear plant/hydrogen plant configurations
  - Modeling of the Next Generation Nuclear Plant (NGNP), a combined nuclear plant/hydrogen plant that will employ a Very High Temperature Gas-Cooled Nuclear Reactor (VHTR) and a high-temperature water-splitting process to produce hydrogen
- FY07
  - Alpha test HyPEP code structure
  - Incorporate high-temperature electrolysis into integrated nuclear plant/hydrogen plant model

Approach

- Progressive code development and cross-checking between development teams and established software packages
    - Identify major systems/components for modeling
    - Establish system parameters and modeling scope
    - Determine overall calculation scheme
    - Develop component models
    - Develop economic and performance optimization models
    - Verify and validate results
- Parallel development of graphical user interface
- Collaborative development across laboratories
    - Idaho National Laboratory (INL)
    - Argonne National Laboratory (ANL)
   - Korea Atomic Energy Research Institute (KAERI)

Technical Accomplishments

- Selected reference NGNP configurations (ANL and INL)
  - General Atomics Sulfur-Iodine and INL high-temp electrolysis methods
  - Parallel electricity and hydrogen production
  - Brayton cycle used for electricity production
  - 600 MWt VHTR with nominal 50 MW hydrogen plants
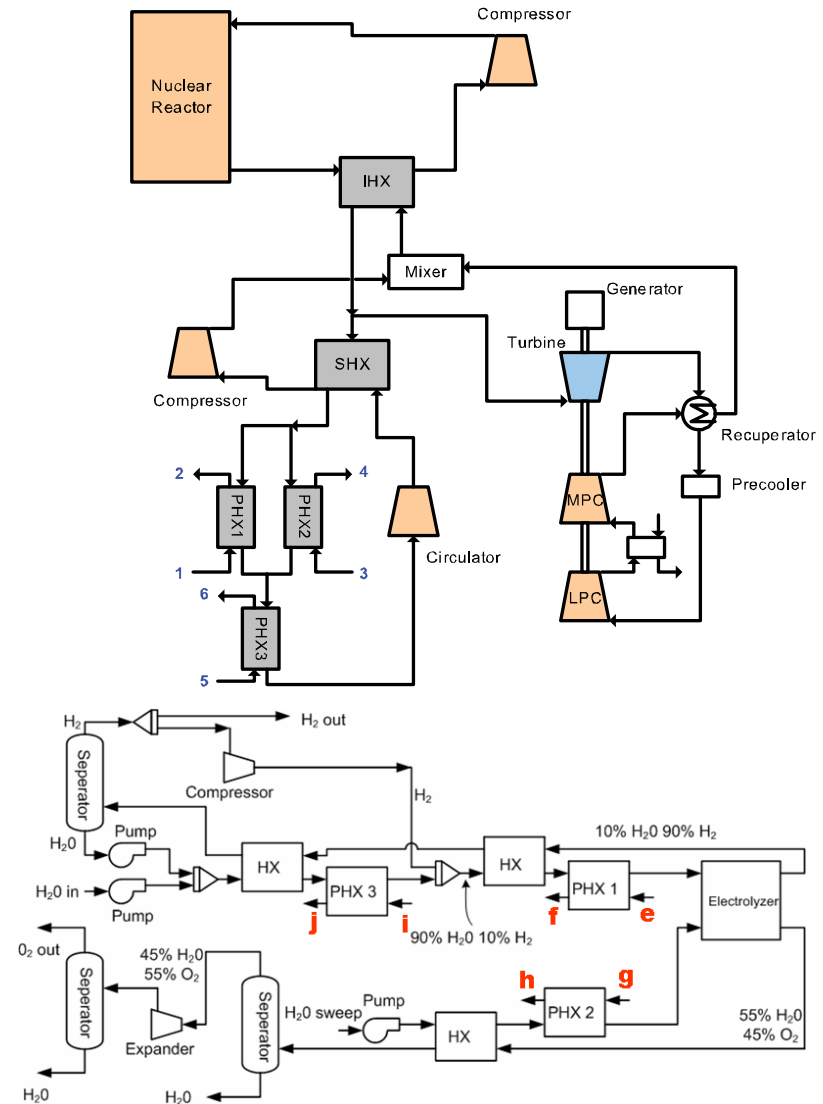
Technical Accomplishments

- Calculation methods devised (KAERI)
  - Network-based thermal/hydraulic system
    - Nodes (volume) connected by links (junction)
  - Field equation formulation
    - Mass and energy conservation
    - Simple flow relations for links
    - Steady-state only

Mass Continuity (for node)
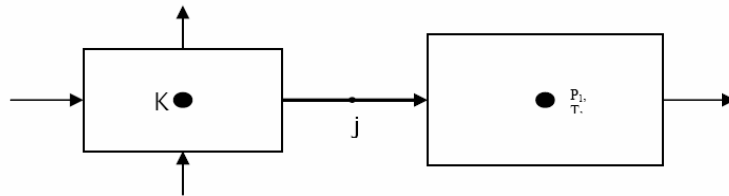
$$V \frac{\partial \rho}{\partial t} = \sum_{j=1}^{N_j} \widetilde{\rho}_j A_j \, u_j + S_m V$$

Energy Continuity (for node)

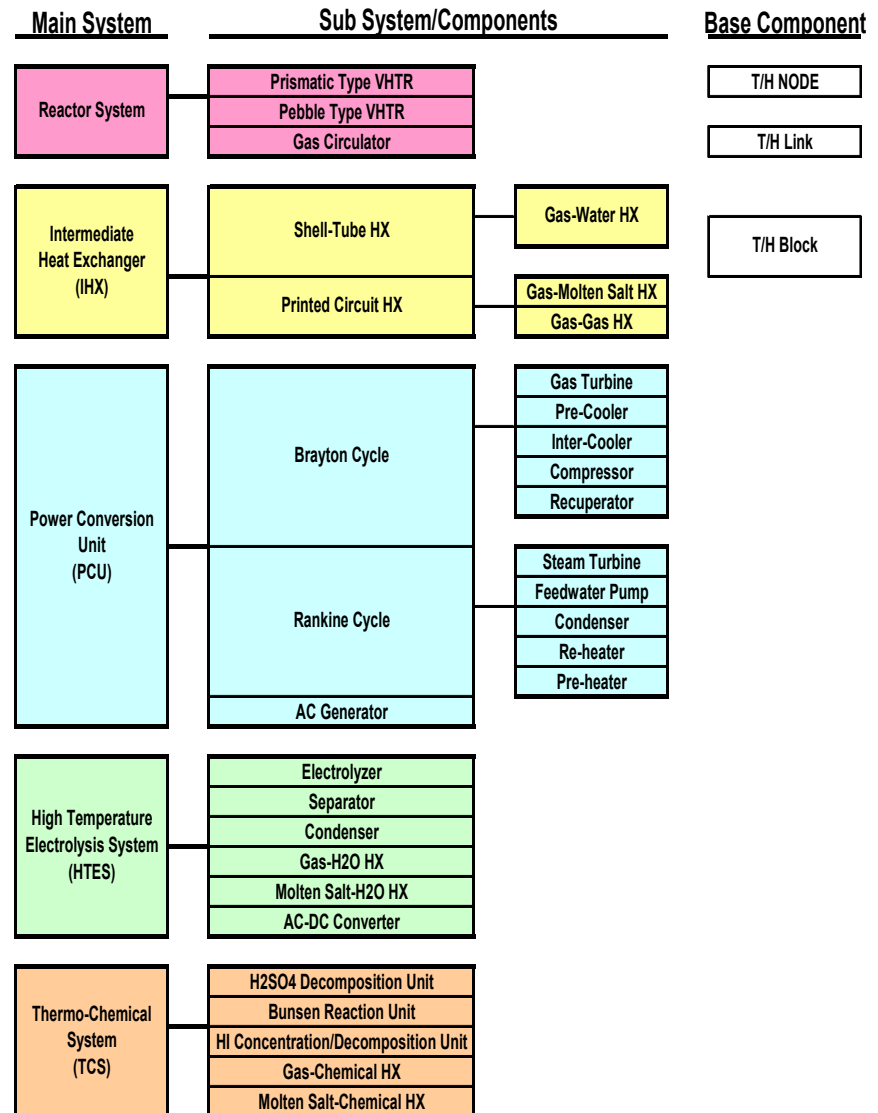$$V \frac{\partial (\rho h)}{\partial t} = \sum_{j=1}^{N_j} \widetilde{\rho}_j \widetilde{h}_j A_j \, u_j + S_h V$$

Flow Relationship (for link j)

$$f_T \frac{\rho u^2}{2} = (P_K - P_L) + \Delta P_{K,source} + \Delta P_{extra}$$
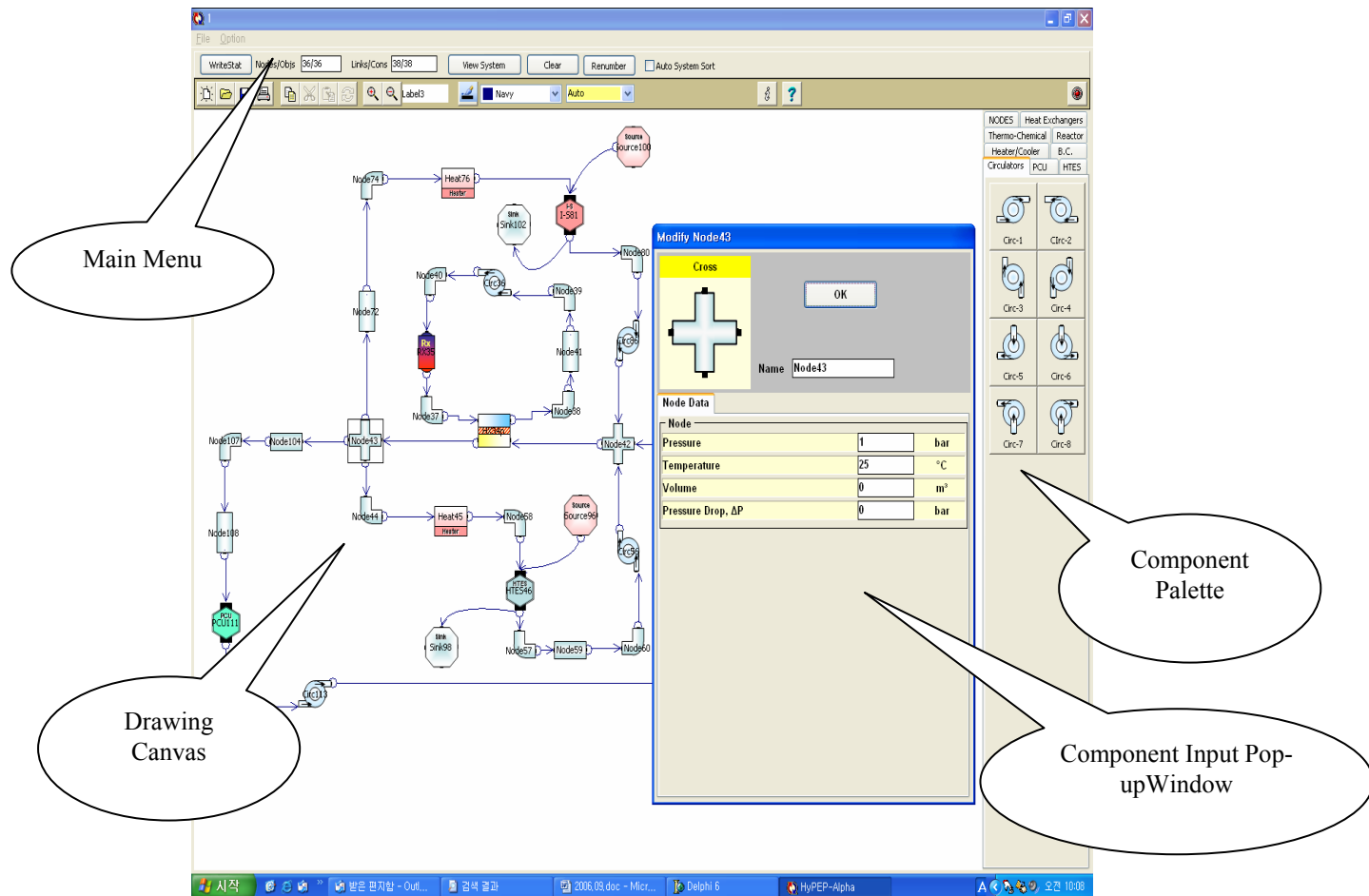
Technical Accomplishments

- Devised overall calculation scheme for HyPEP (KAERI)
    - Node-link-block
    - Hierarchical arrangement of sub-units
    - Examined use of Fortran, C#, Visual Basic and Delphi
        - Selected Delphi 2006 for its excellent object-oriented programming structure and compatibility with Win32 and .NET environments

Main System	Sub System/Components		Base Component

Reactor System
- Prismatic Type VHTR
- Pebble Type VHTR
- Gas Circulator

Intermediate Heat Exchanger (IHX)
- Shell-Tube HX — Gas-Water HX
- Printed Circuit HX — Gas-Molten Salt HX, Gas-Gas HX

Power Conversion Unit (PCU)
- Brayton Cycle — Gas Turbine, Pre-Cooler, Inter-Cooler, Compressor, Recuperator
- Rankine Cycle — Steam Turbine, Feedwater Pump, Condenser, Re-heater, Pre-heater
- AC Generator

High Temperature Electrolysis System (HTES)
- Electrolyzer
- Separator
- Condenser
- Gas-H2O HX
- Molten Salt-H2O HX
- AC-DC Converter

Thermo-Chemical System (TCS)
- H2SO4 Decomposition Unit
- Bunsen Reaction Unit
- HI Concentration/Decomposition Unit
- Gas-Chemical HX
- Molten Salt-Chemical HX

Base Component
- T/H NODE
- T/H Link
- T/H Block

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Technical Accomplishments

- Development of graphical user interface (KAERI)

Technical Accomplishments

- Verification (development of comparison models)
  - Detailed modeling and parametric studies of high-temperature electrolysis reference design using HYSYS by Aspentech (INL)
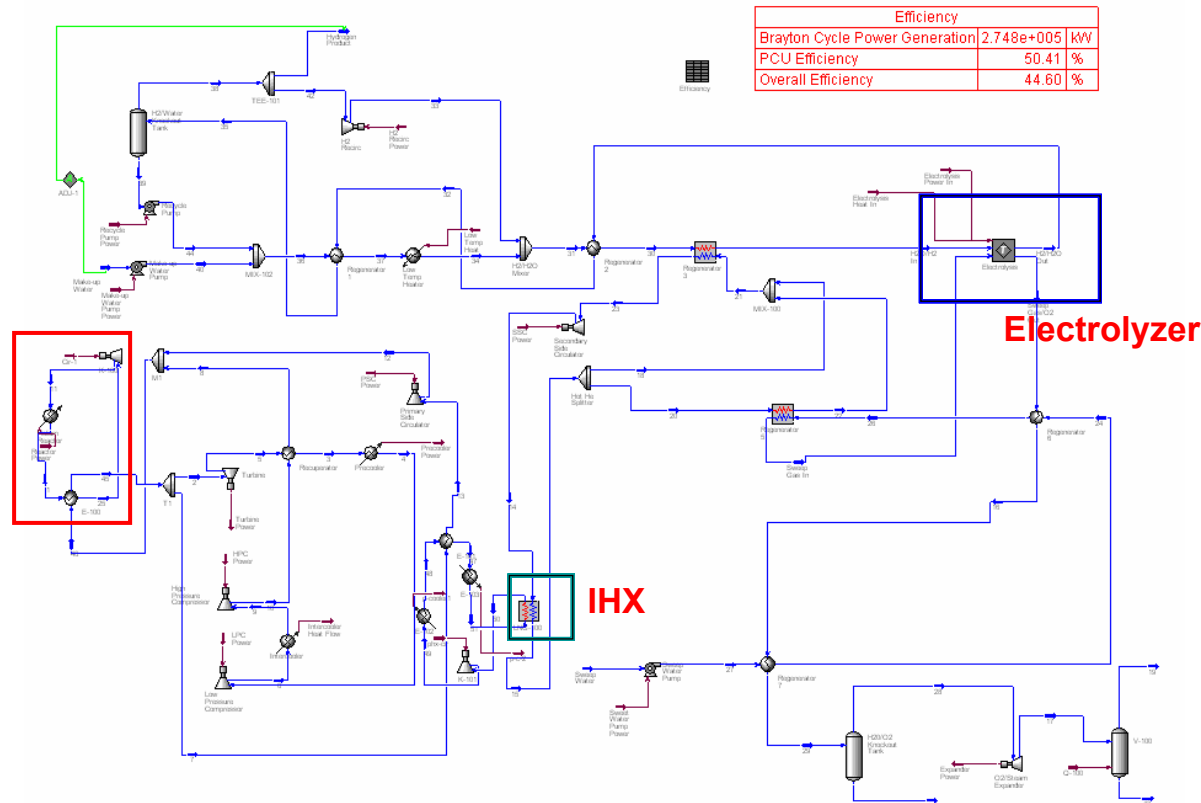
Technical Accomplishments

- Verification (development of comparison models)
  - Gas-Pass/H model also used to examine system configurations (ANL)
    - Code modified to accommodate temperature dependent fluid densities
    - Network-based representation parallels that of HyPEP
    - Gas-Pass/H allows use of time-dependent (non-steady-state) equations, and so might be used in the future for examination of start-up, shutdown, off-normal, and control system strategies
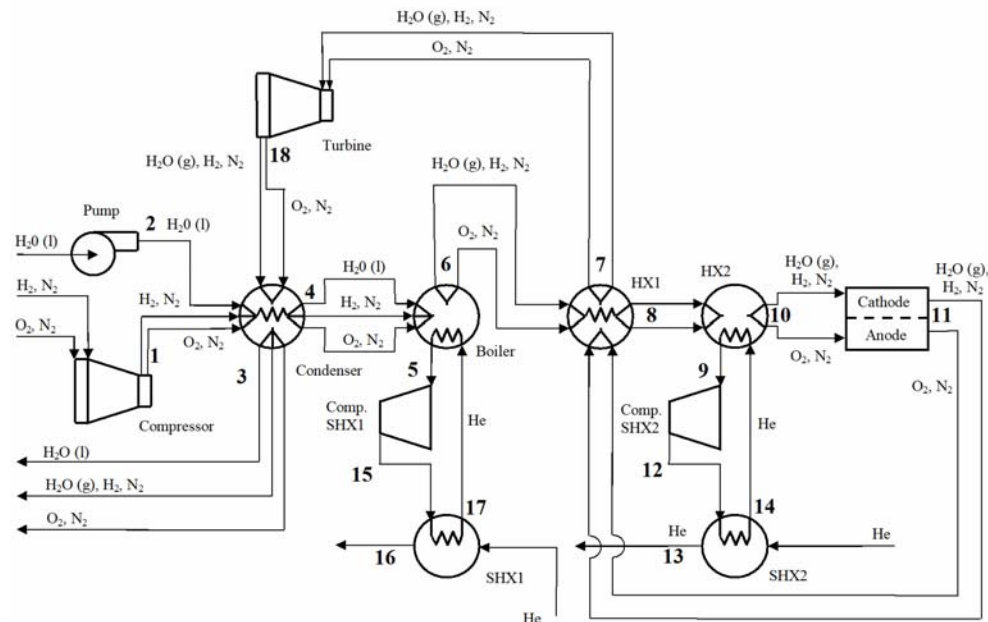
Technical Accomplishments

- HyPEP alpha version is undergoing testing in FY07 (KAERI)
  - Node-link-block: basic T/H components
  - Sink,source: boundary condition (node)
  - Fill, drain: boundary condition (link)
  - Heat exchanger: derived (node, block)
  - Circulator: simple model
  - Nuclear Reactor: simple model
  - Hydrogen plants: black box models (node-based)
  - Power conversion unit: black box models (node-based)
  - Very limited analysis capability; only basic or conceptual problems with simple layouts can be handled at this time

Future Work

- Remainder FY07
  - Complete parametric studies of high-temperature electrolysis configuration (INL)
    - Changes in pressures, parallel versus serial, heat transfer fluids and fluid conditions
  - Continue to develop non-steady-state integrated models using GAS-PASS/H (ANL)
  - Prepare HyPEP model for beta-testing (KAERI)
  - Release HyPEP to INL and ANL for validation/verification
  - Release initial HyPEP User Manual

Future Work

- FY08
  - Incorporation of most recent General Atomics Sulfur-Iodine reference flow sheet and chemical kinetics data into integrated HYSYS model (INL)
  - Development of dynamic integrated system models for configurations of interest using GAS-PASS/H and cross-validation of models against HyPEP and HYSYS (ANL)
  - Beta-testing of HyPEP (ANL, INL, KAERI)
  - Incorporation of basic economic and component sizing modules (KAERI)
  - Public release of fully capable HyPEP tool (KAERI)
    - Updated User's Manual
    - Models and Correlations Manual

Summary

- HyPEP – <u>Hy</u>drogen <u>P</u>roduction <u>E</u>fficiency Calculation <u>P</u>rogram

- I-NERI Project between ANL, INL, and KAERI

- Within Year 2 of a 3-year Project

- Steady-state integrated model of NGNP includes INL high-temp electrolysis and soon General Atomics Sulfur-Iodine Method

- Currently undergoing alpha-testing

- Will undergo beta testing in FY08

- Finished software will provide easy-to-use validated program for calculating energy efficiencies and relative costs of different NGNP configurations